Work by Olof Widlund's group
a.k.a. NYU update

and

Fast Solvers and Schwarz Preconditioners
for high order discretizations
of a Maxwell model problem

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Our group

Paulo Goldfeld
(Balancing Neumann-Neumann)

Bernhard Hientzsch
(Maxwell & more)

Jing Li
(FETI-DP for CFD)

Josè Cal Neto
(FETI-DP for 4th order)

Olof Widlund
("everything")

Paulo Goldfeld: Balancing Neumann-Neumann

- Balancing Neumann-Neumann for

  - Incompressible Elasticity
  - Compressible Elasticity
  - Stokes
  - Navier-Stokes by Newton-Krylov (in progress)
  - Neumann-Neumann-like nonlinear preconditioner for global nonlinear problem (planned)

- Implemented in PETSc, run on large clusters such as Chiba City.

- Question: in PETSc LU for local Stokes or incompressible Elasticity breaks down with standard ordering, tricks needed. Other direct solvers (SuperLU) ? Possibly adapted for saddle point structure?

- Most CPU time: factorization of the local problems at start-up. Iterative methods do not seem to be a viable alternative.

- Theory by Widlund and Pavarino

Jing Li: FETI-DP

- FETI-DP for

  - Stokes

  - Oseen

  - Navier-Stokes by Newton-Krylov

  - FETI-like preconditioner for global nonlinear problem (planned)

- Sequential code in C++, implementation in PETSc planned.

- Theory by Li (2 short papers).

Olof Widlund

- Theory for

  - Neumann-Neumann
  - FETI-DP methods (paper with Klawonn and Dryja, to appear)
  - Mortar methods
  - ...

- for

  - Stokes (paper just accepted)
  - Incompressible and Compressible Elasticity (almost complete paper)
  - $H(\mathrm{div})$, $H(\mathbf{curl})$ (a few years ago)
  - ...

- Nonlinear preconditioners (with: Xiao-Chuan Cai).

Previous work in our group for $H(\text{div})$ and $H(\mathbf{curl})$

- Lower order (usually first) Nédélec elements

- Toselli: Overlapping Schwarz for $H(\mathbf{curl})$ (2D, 3D)

- Toselli and Hiptmair: Multilevel for $H(\text{div})$ and $H(\mathbf{curl})$

- Toselli, Widlund, and Wohlmuth: Iterative substructuring for $H(\mathbf{curl})$ (2D)

- Toselli: Neumann-Neumann for $H(\mathbf{curl})$

- Toselli and Klawonn, Toselli and Rapetti: FETI for $H(\mathbf{curl})$

- Wohlmuth, Toselli, and Widlund: Iterative substructuring for $H(\text{div})$ (2D,3D)

Bernhard Hientzsch: High order Maxwell

- Fast direct solvers for rectangular domains.

- Direct substructuring methods for domains composed out of rectangular elements

- Helmholtz decomposition solvers

- Overlapping Schwarz methods

- Iterative substructuring methods (in progress), threedimensional implementation (in progress), ...

- Codes in MATLAB and some in C using MPI for parallelization.

- Theory by Hientzsch extending analysis by Toselli.

$$(\alpha u, v) + (\beta \, \mathbf{curl} \, u, \mathbf{curl} \, v) = f(v)$$

- Spectral Elements: Spectral Methods (high accuracy, special structure) + Finite Element Methods (geometric flexibility) + Numerical Integration

- Discretization $Ku = Mf$ has block tensor product structure, allows fast computation of $w = Kv$, and, for rectangular domains, <u>fast direct solvers</u> . Those are needed as local solvers and global coarse solvers.

- Domain Decomposition approach leads to quasi-optimal and parallel methods for more complicated and larger examples.

- Preconditioners seem to be relatively robust with respect to moderate deformation of the geometry and mesh

Spectral Nédélec Elements for H(curl)

- H^1-conforming elements: spurious eigenvalues and unphysical continuity conditions

- Nédélec [Num. Math. '80, '86]: H(curl) conforming elements, d.o.f.: edge, face and interior moments; Monk and others: hp-, hN-extension

- Ben Belgacem and Bernardi [Math. Comp. '99]: Spectral element method for Maxwell's equation.

- We use spectral element type nodal degrees of freedom, variable order Gauss-Lobatto-Legendre quadrature, only tangential continuity.

- We construct mapping between spectral element and Nédélec degrees of freedom for different degrees, and analyze the interpolation properties and the stability of the local splitting for the Nédélec interpolant.

The model problem

- Maxwell in E:

$$\epsilon \partial_t^2 \mathbf{E} + \sigma \partial_t \mathbf{E} + \mathbf{curl}\left(\frac{1}{\mu} \mathbf{curl}\, \mathbf{E} \right) = \partial_t \mathbf{j}_i$$

- Implicit time integration:

$$\alpha \mathbf{u} + \mathbf{curl}(\beta \, \mathbf{curl}\, \mathbf{u}) = f$$

- Variational form:

$$(\alpha \mathbf{u}, \mathbf{v})_{L^2} + (\beta \, \mathbf{curl}\, \mathbf{u}, \mathbf{curl}\, \mathbf{v})_{L^2} = \mathbf{f}(\mathbf{v})$$

- GLL quadrature:

$$(\alpha \mathbf{u}, \mathbf{v})_{GLL} + (\beta \, \mathbf{curl}\, \mathbf{u}, \mathbf{curl}\, \mathbf{v})_{GLL} = \mathbf{f}_{GLL}(\mathbf{v})$$

- Discretized form on one element (2D):

$$\begin{pmatrix} M_1^x \otimes A^y & B^x \otimes C^y \\ B^{x,T} \otimes C^{y,T} & A^x \otimes M_2^y \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \begin{pmatrix} \tilde{f}_1 \\ \tilde{f}_2 \end{pmatrix}$$

- Subassembling on rectangular arrangement with appropriate degrees with tangential continuity gives system matrix of the same structure

Modelproblem in 3D

Stiffness matrix has the form:

$$\begin{pmatrix} C_{11} & C_{12} & C_{13} \\ C_{21} & C_{22} & C_{23} \\ C_{31} & C_{32} & C_{33} \end{pmatrix}$$

$$
\begin{aligned}
C_{11} &= M_x \otimes (\alpha M_y \otimes M_z + \beta(K_y \otimes M_z + M_y \otimes K_z)) \\
C_{22} &= P^{xyz}_{yxz}(M_y \otimes (\alpha M_x \otimes M_z + \beta(K_x \otimes M_z + M_x \otimes K_z)))P^{yxz}_{xyz} \\
C_{33} &= (\alpha M_x \otimes M_y + \beta(K_x \otimes M_y + M_x \otimes K_y)) \otimes I_z
\end{aligned}
$$

$$
\begin{aligned}
C_{12} &= -D_x \otimes \tilde{D}_y \otimes M_z \\
C_{13} &= -D_x \otimes M_y \otimes \tilde{D}_z \\
C_{21} &= -\tilde{D}_x \otimes D_y \otimes M_z \\
C_{23} &= -M_x \otimes D_y \otimes \tilde{D}_z \\
C_{31} &= -\tilde{D}_x \otimes M_y \otimes D_z \\
C_{32} &= -M_x \otimes \tilde{D}_y \otimes D_z
\end{aligned}
$$

with M one-dimensional mass matrix, K one-dimensional Laplace, D and $\tilde{D}$ combinations of derivative and mass matrices, P transposition of the 3D array.

Algorithms:

- Direct block tensor solver

- Direct substructuring solver

- Algorithmic components for DDM

- Overlapping Schwarz Preconditioners

- Helmholtz decomposition solvers

Direct block tensor solver (2D)

- Eliminate one component in block tensor product system in both components to obtain generalized Sylvester matrix equation in one component

$$(A \otimes B + C \otimes D)u_i = f$$

- Solve Sylvester matrix equation by:

  - Transformation to special form, use fast diagonalization method [Lynch et al, Num. Math '64] (sometimes ill-conditioned eigensystems)

  - Work on generalized Sylvester equation, use Hessenberg or Schur forms [Gardiner et al, ACM TOMS '92, Kågström, Poromaa ACM TOMS '96]

- Setup takes $O(n^3)$ time, per right hand side $O(n^{d+s})$ with $s \in [0, 1]$ depending on the fast matrix-matrix multiplication used.

Direct substructuring solver

- Form local Schur complements

- Subassemble local Schur complements to Schur complement system on tangential components on element interfaces

- Subassemble right hand side for the Schur complement system on the interfaces

- Solve the Schur complement system on the interface

- Compute interior values in each spectral element by one tangential value boundary problem solve per element

Domain decomposition methods: algorithmic components

- Compute residual

- Solve local problems with different boundary conditions

- Solve low-order global problem

For direct and iterative substructuring methods :

- Form local Schur complement

- Compute right hand side for Schur complement system

- Apply local Schur complement or its inverse to a vector

# Overlapping Schwarz method: implementation in 2D

- Define overlapping subregions $\Omega'_{i,\delta} \subset \Omega$. Several ways: extending coarse elements or subdomains, or vertex-centered. Most of our computations: 2×2 vertex centered domain decomposition.
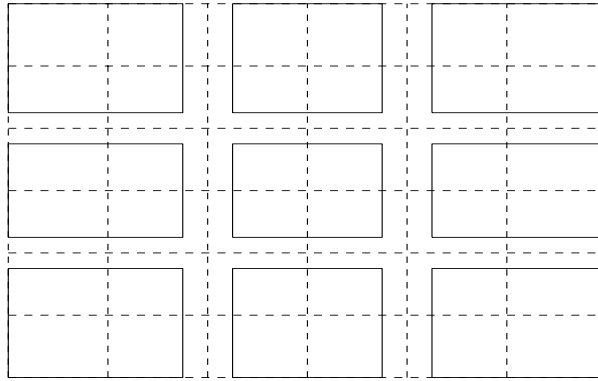
- Local spaces and solvers: take basis functions associated to GLL points in $\Omega'_{i,\delta}$ (submatrix) . Elementwise-overlap: standard tangential value solve on 2x2 elements. $V_i \subset \mathbb{ND}_N^{II,0}(T_H)$.

- Coarse space: low-order (spectral) Nédélec elements. $V_0 = \mathbb{ND}_{N_0}^{II,0}(T_H)$

Overlapping Schwarz method: overlapping subregions

Vertex centered domain decomposition:
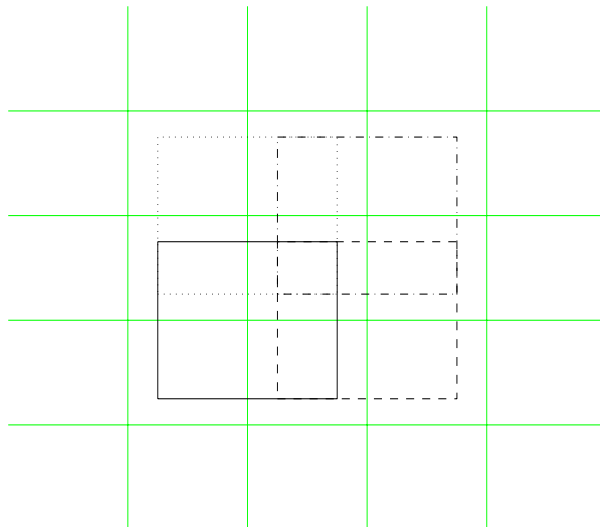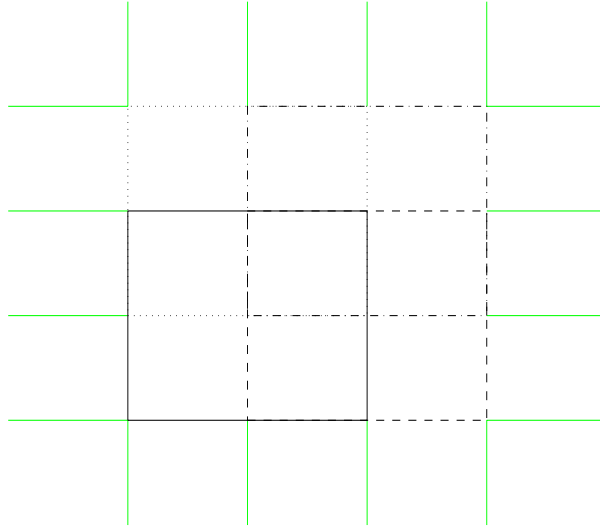
Helmholtz decomposition solvers

- $f = (\alpha I + \beta \, \mathbf{curl}\,\mathbf{curl})u$

- Use $f = cf(f) + df(f) = \mathbf{grad}\, q + \mathbf{curl}\,\Phi$, q scalar, Φ scalar (2D), vector (3D)

- On $cf(u)$ operates as αI, on $df(u)$ operates as $\alpha I + \beta \Delta$.

- Suggests method like: compute $cf(f)$ (Laplace), compute $cf(u) = \frac{1}{\alpha} cf(f)$, find $df(u)$ by solving Helmholtz-type equation on components (2D,3D) or potential (2D) with appropriate b.c.

- For some boundary conditions (e.g., natural), this gives in 2D a spectrally convergent solver (numerically); for others (f.i. essential = tangential), only algebraic convergence (corner and edge effects) which can be improved but not (yet?) made exponential

Some numerical examples

- Rectangular domain: convergence, some timings

- L-shape domain: direct substructuring solver

- Overlapping Schwarz Preconditioners: results for one- and two-level methods

Direct solvers: Rectangular domain

5×5 spectral elements, degree: ($N \times N$, $N \times N$). Different numerical integrations for the mass matrix: exact integration and diagonal mass matrix. Block tensor and Interface Schur complement solvers.
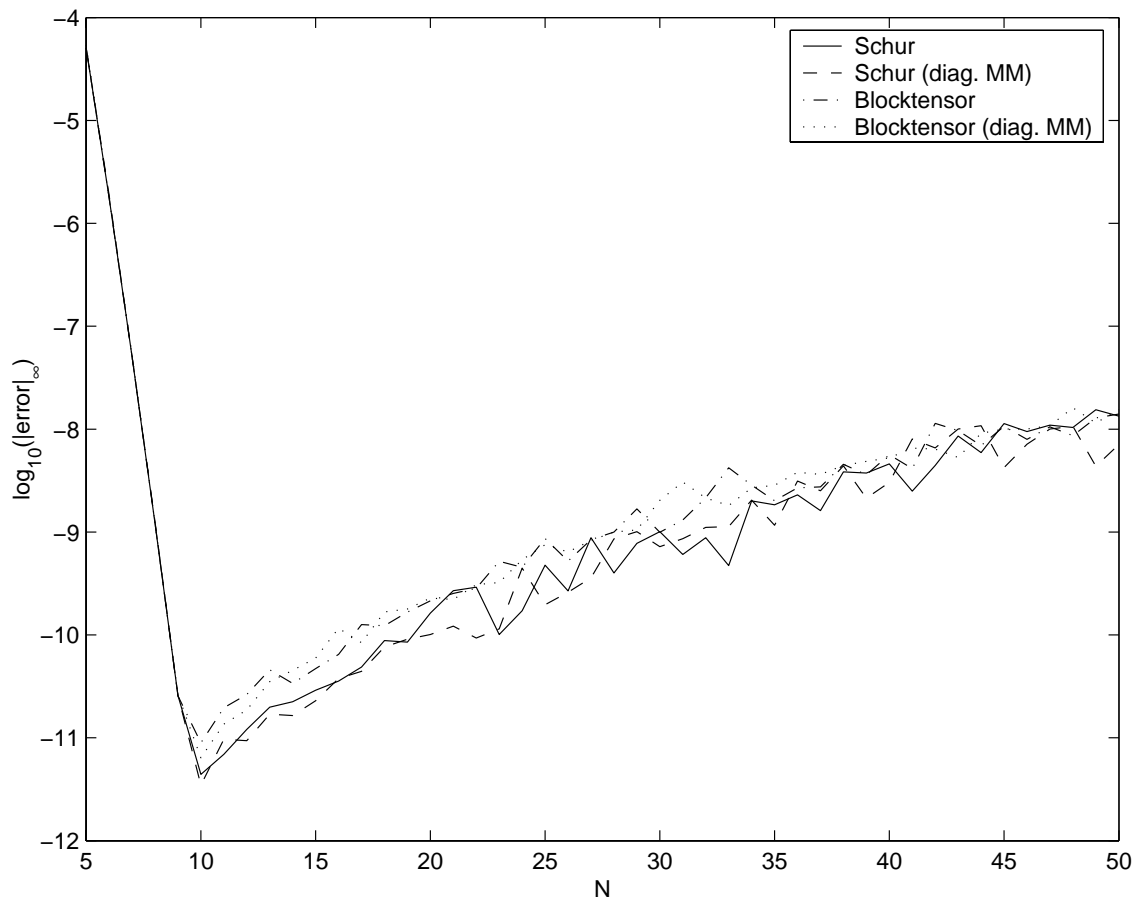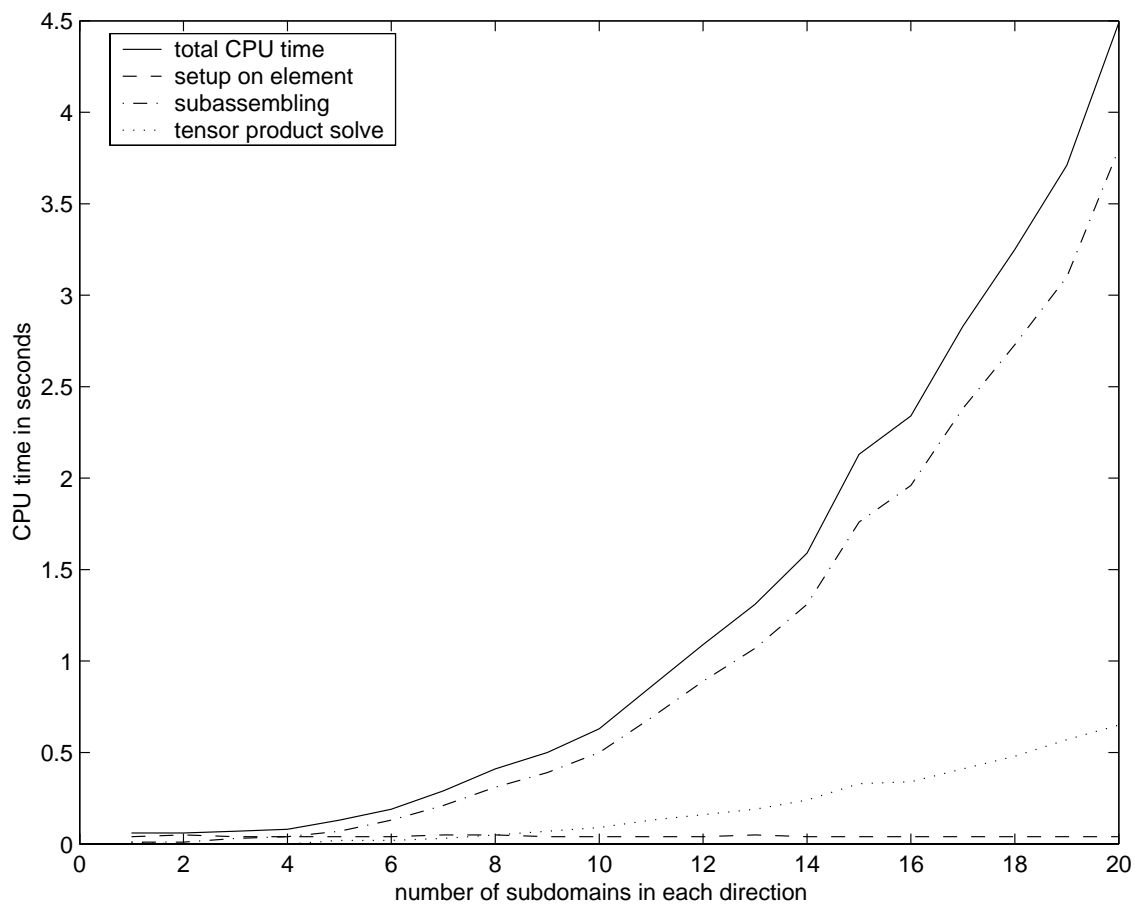
Direct methods: Timings, block tensor solver

5×5 spectral elements of degree N. Exact element matrices.
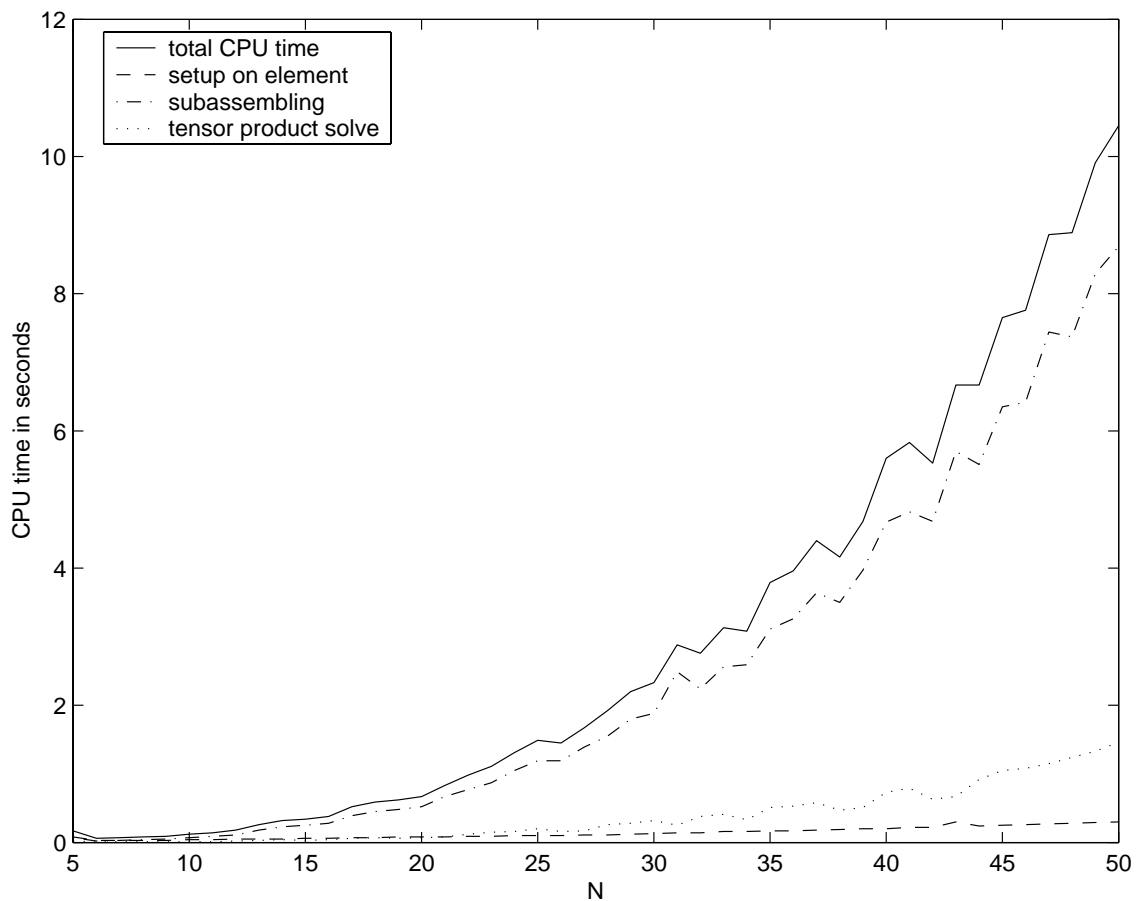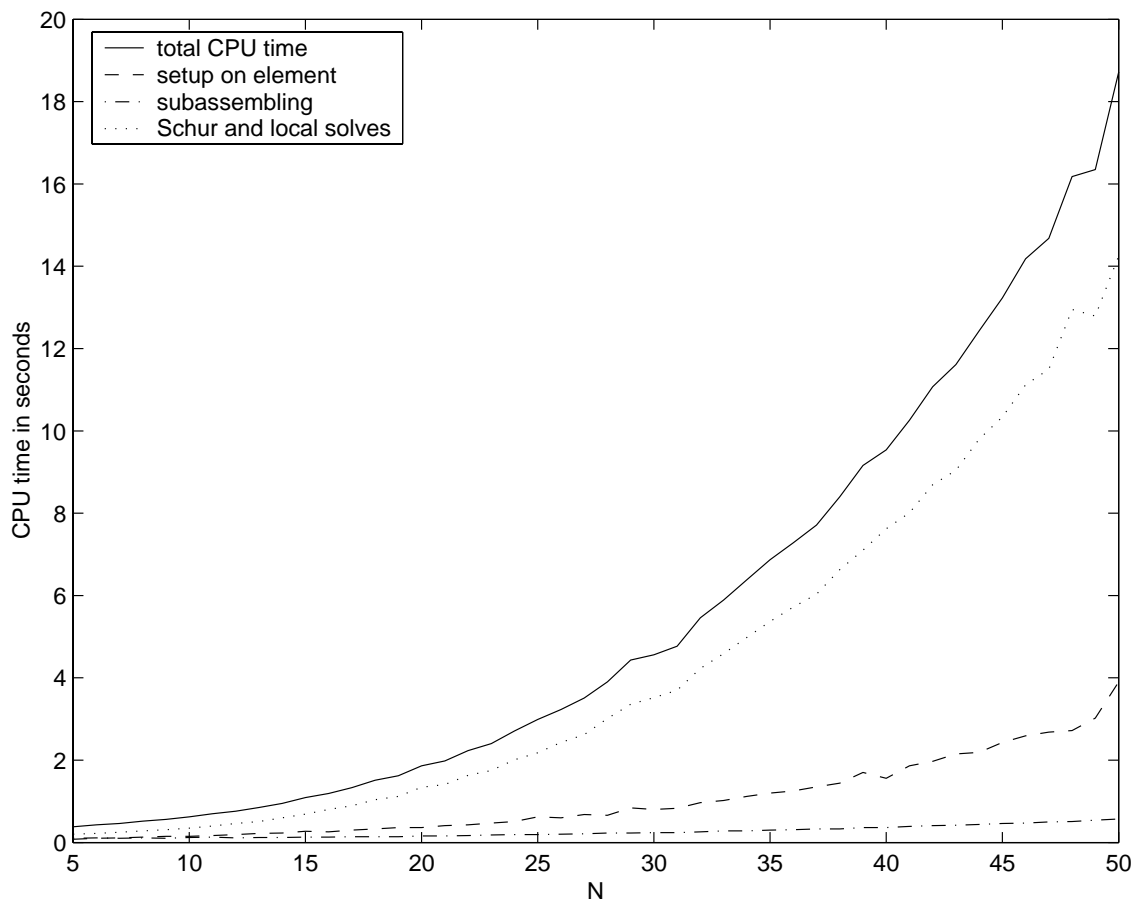
Direct methods: Timings, block tensor solver

$M \times M$ spectral elements of degree 10×10.
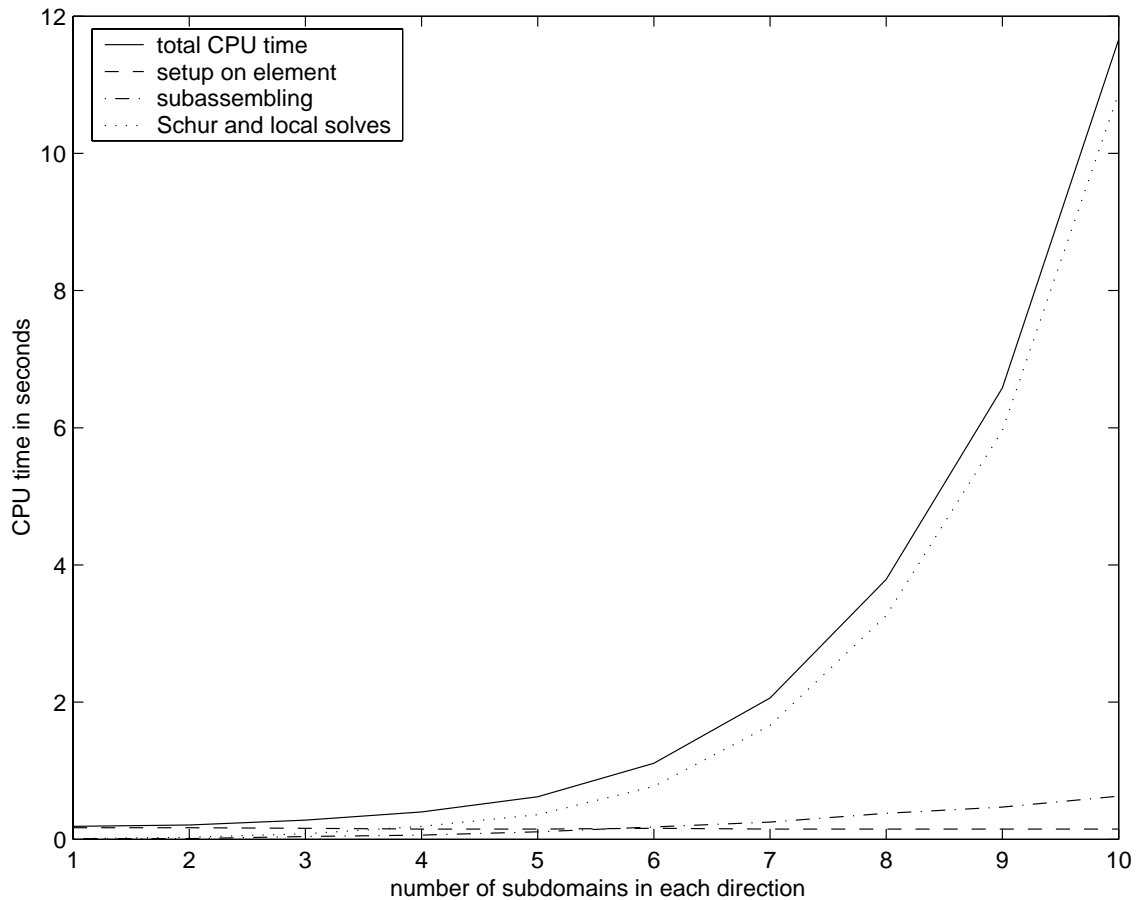Exact element matrices.

Direct methods: Timings, Schur interface solver

5×5 spectral elements of degree N. Exact element matrices.

Direct methods: Timings, Schur interface solver

$M \times M$ spectral elements of degree 10×10. Exact element matrices.

# Direct methods: Summary of comparison (rectangular domain)

- Increasing N: in exponential convergence indistinguishable, for larger N Schur solvers slightly more accurate.

- Schur solver: out of memory at $M = 10$ and $N > 10$. Tensor solver runs in memory for much larger examples.

- Tensor solver: most time in subassembling, computing eigenbases and inverses. Actual solve is very fast ($< 2s$ for $N = 50$, $M = 5$, $< 1s$ for $M = 10$, $N = 10$)

- Schur solve: most time in computing rhs, solving Schur system and local systems. (Needs to be done for each rhs.)

- Block tensor solver twice as fast, per rhs seven times as fast for $N = 50$, $M = 5$. 20 times as fast at $M = 10$, $N = 10$, per rhs more than 100 times as fast.

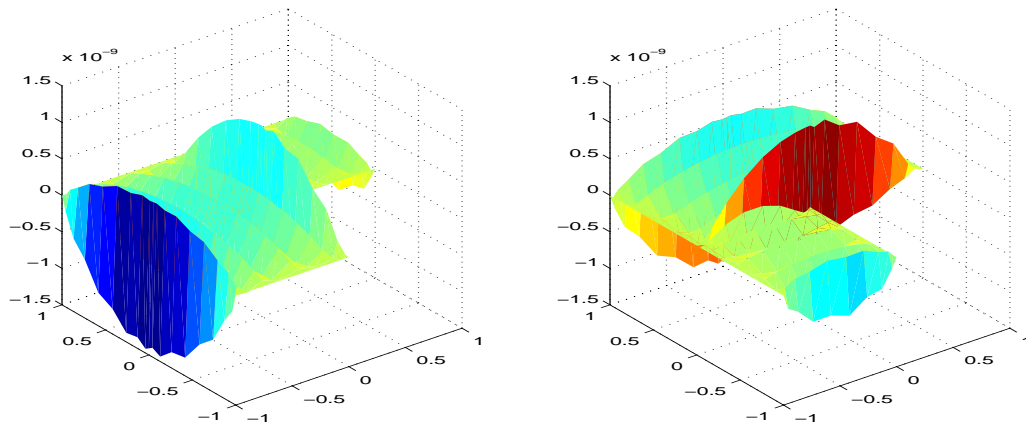# Schur interface solver on L-shaped domain

Exact solution:
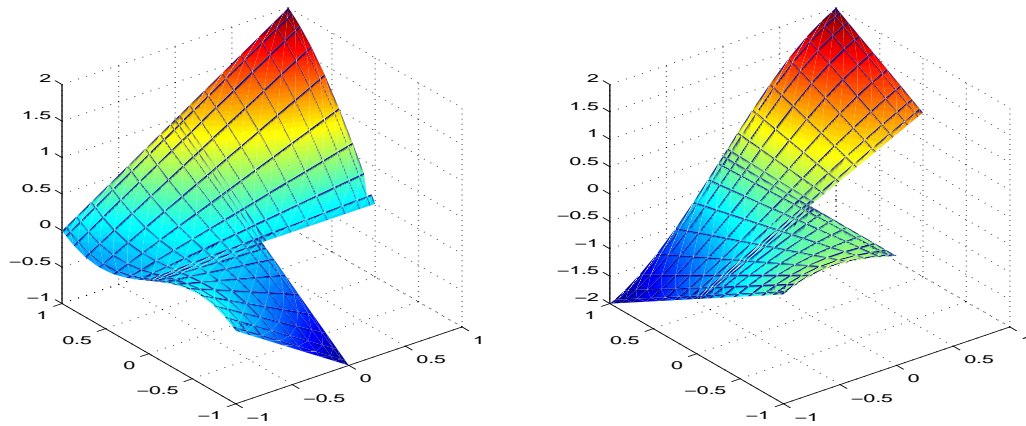
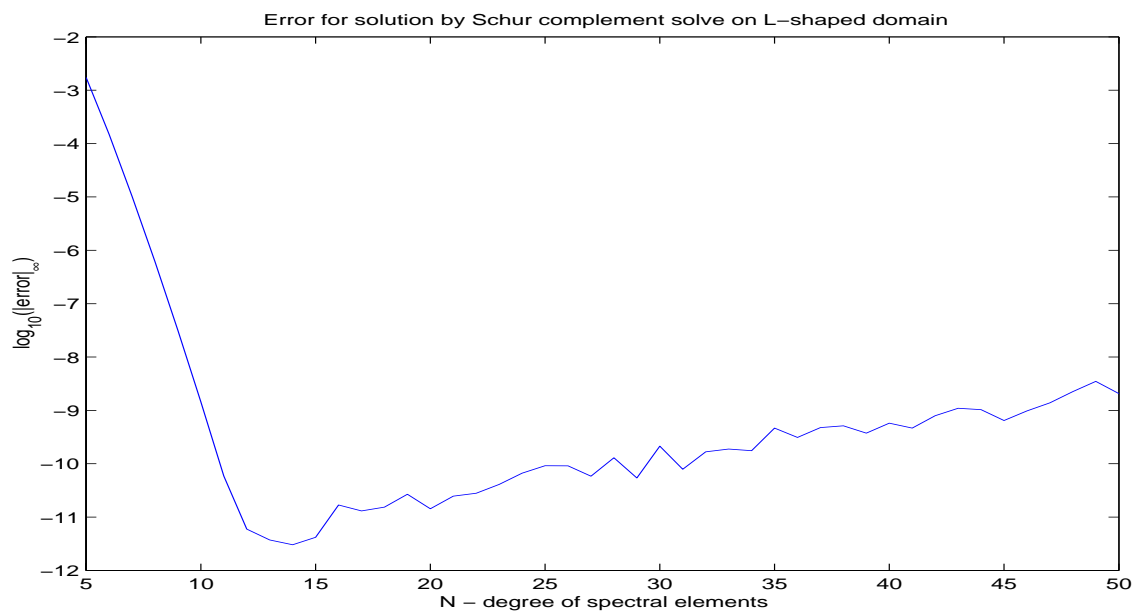GLL grids with interface degrees of freedom marked by 'x', for degree 10:
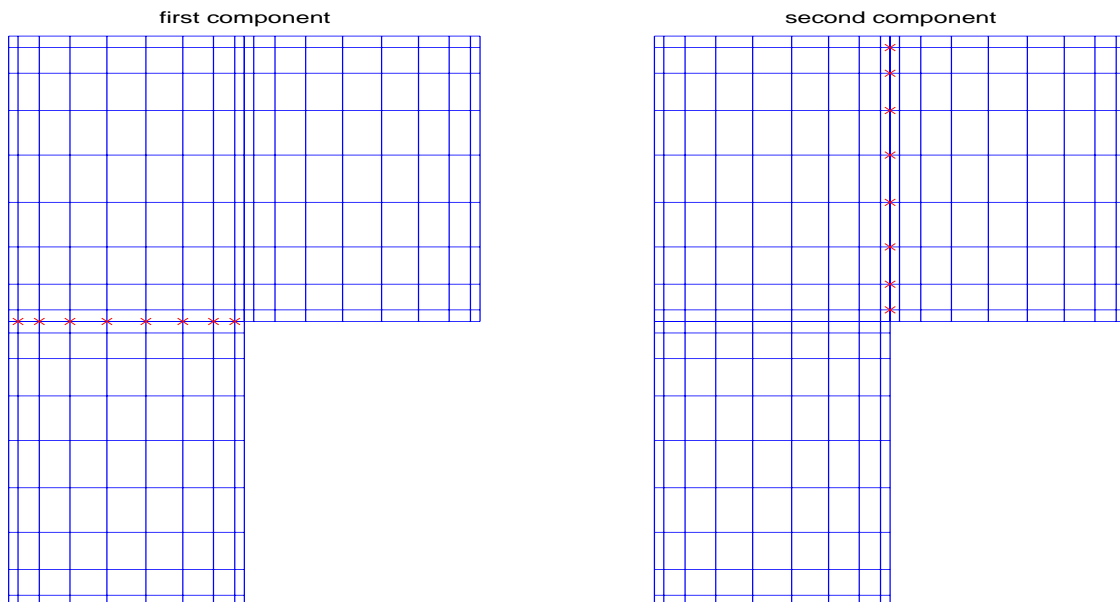
Schur interface solver on L-shaped domain

Error of the solution, for degree 10:

Maximum error of the solution over degree N of the spectral elements:

Overlapping Schwarz method:
Numerical results in 2D

Comparison of different methods for $\alpha = \beta = 1$, $M = N = 10$:

# of levels	iter	$\kappa_{est}(K)$	$\|\text{error}\|_\infty$	t_{CPU} in s
(no pc)	3580	1.44e+06	5.73e-05	448.6
one	31	38.2	3.21e-06	7.6
two ($N_0 = 2$)	15	4.93	3.78e-06	3.8
two ($N_0 = 3$)	15	4.52	9.95e-07	3.8
two ($N_0 = 4$)	15	4.51	9.48e-07	3.9
two ($N_0 = 5$)	14	4.49	1.88e-06	3.8

Overlapping Schwarz method: Results for one-level methods

One-level method, using 2×2 vertex centered domain decomposition, varying number of spectral elements of degree 10×10:
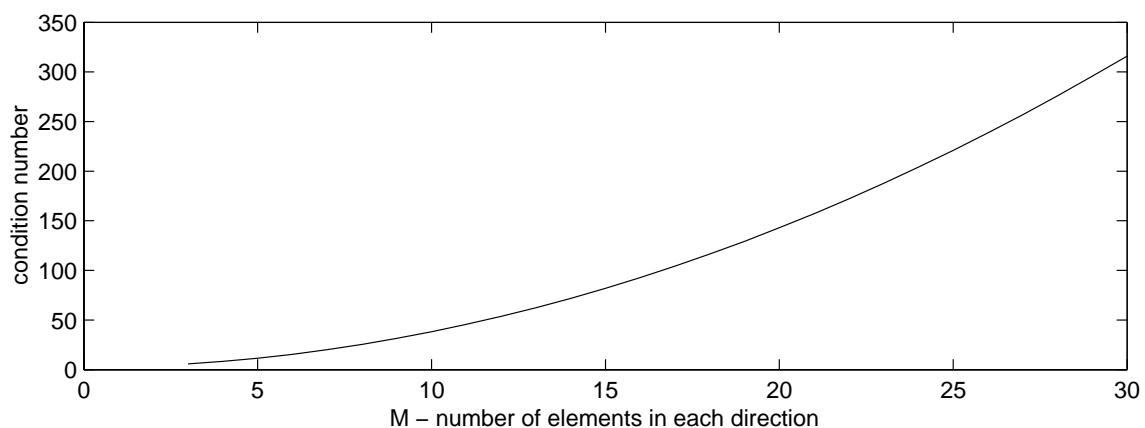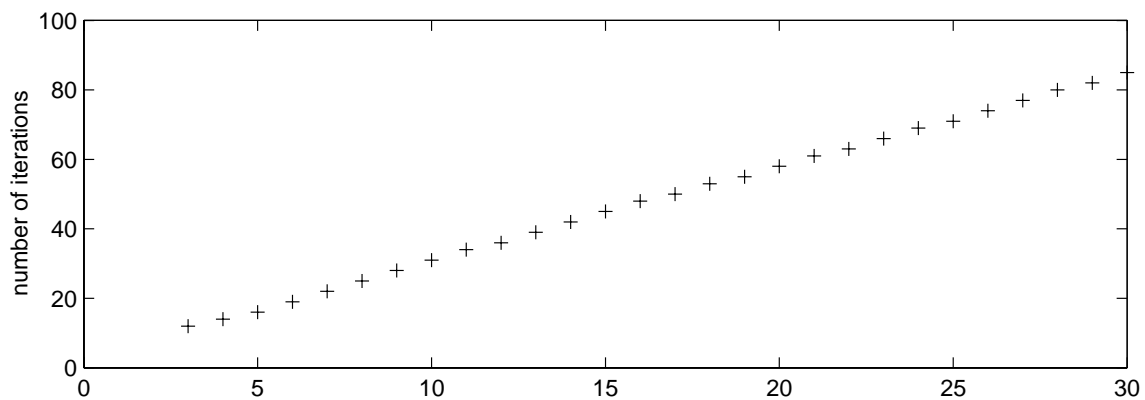
Comparison of different methods for the 2×2 vertex centered domain decomposition for $\alpha = \beta = 1$, $N = 10$.

| # of levels	iter	$\kappa_{est}(K)$	$\|\text{error}\|_\infty$	t_{CPU} in s
$M = 20$				
one	58	142.9	2.05e-06	74.4
two ($N_0 = 2$)	15	4.84	1.46e-06	19.6
two ($N_0 = 3$)	14	4.84	1.49e-06	18.9
two ($N_0 = 4$)	15	4.85	5.56e-07	20.7
$M = 30$				
one	85	316.0	1.59e-06	251
two ($N_0 = 2$)	15	4.91	1.03e-06	47.2
two ($N_0 = 3$)	15	4.93	3.74e-07	47.7
two ($N_0 = 4$)	15	4.93	3.11e-07	49.7
$M = 40$				
two ($N_0 = 2$)	15	4.95	7.24e-07	98.3
two ($N_0 = 3$)	15	4.96	2.66e-07	102.2
two ($N_0 = 4$)	15	4.96	2.15e-07	106.0

Overlapping Schwarz method: Results for two-level method

Two-level method, using 2×2 vertex centered domain decomposition, varying number of spectral elements, degree 10×10, $N_0 = 3$.
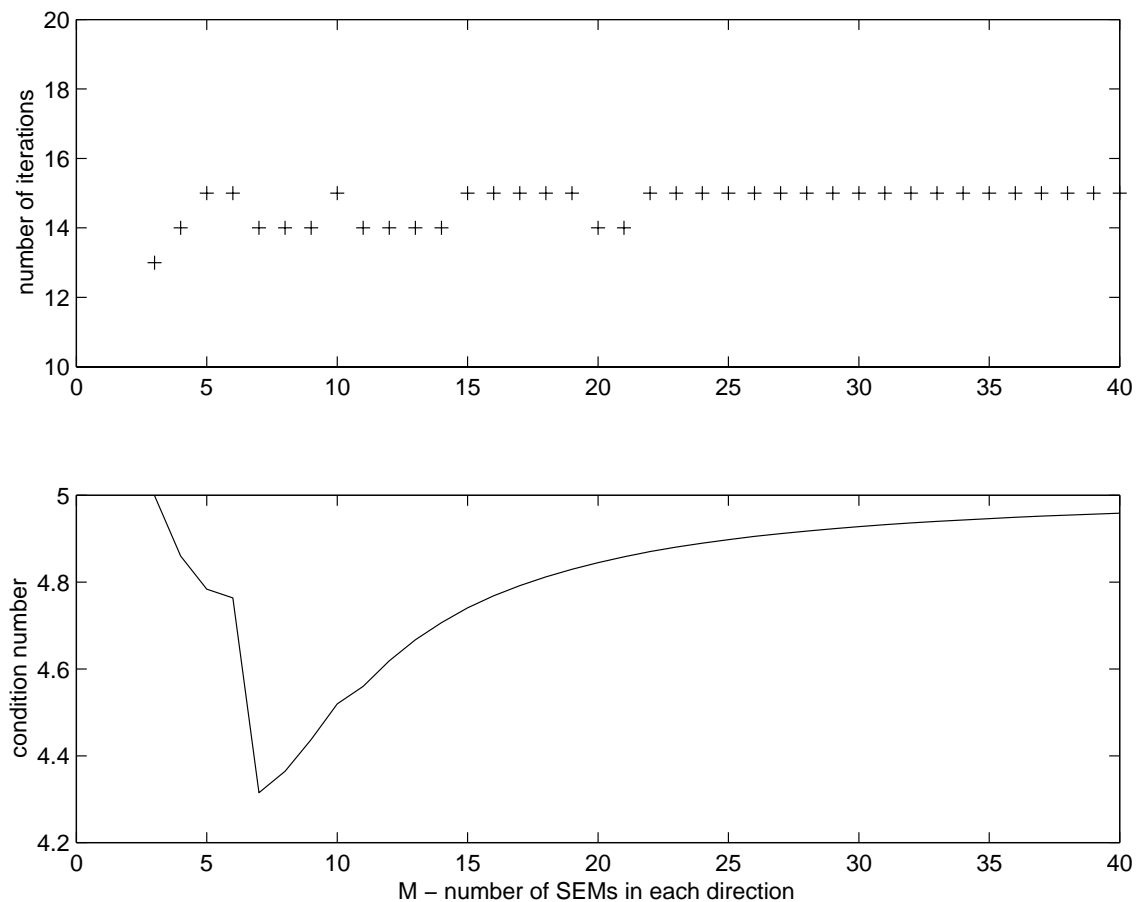
Overlapping Schwarz method: Results for two-level method

Two-level method, using 2×2 vertex centered domain decomposition, 10×10 spectral elements, degree $N \times N$, $N_0 = 2$.
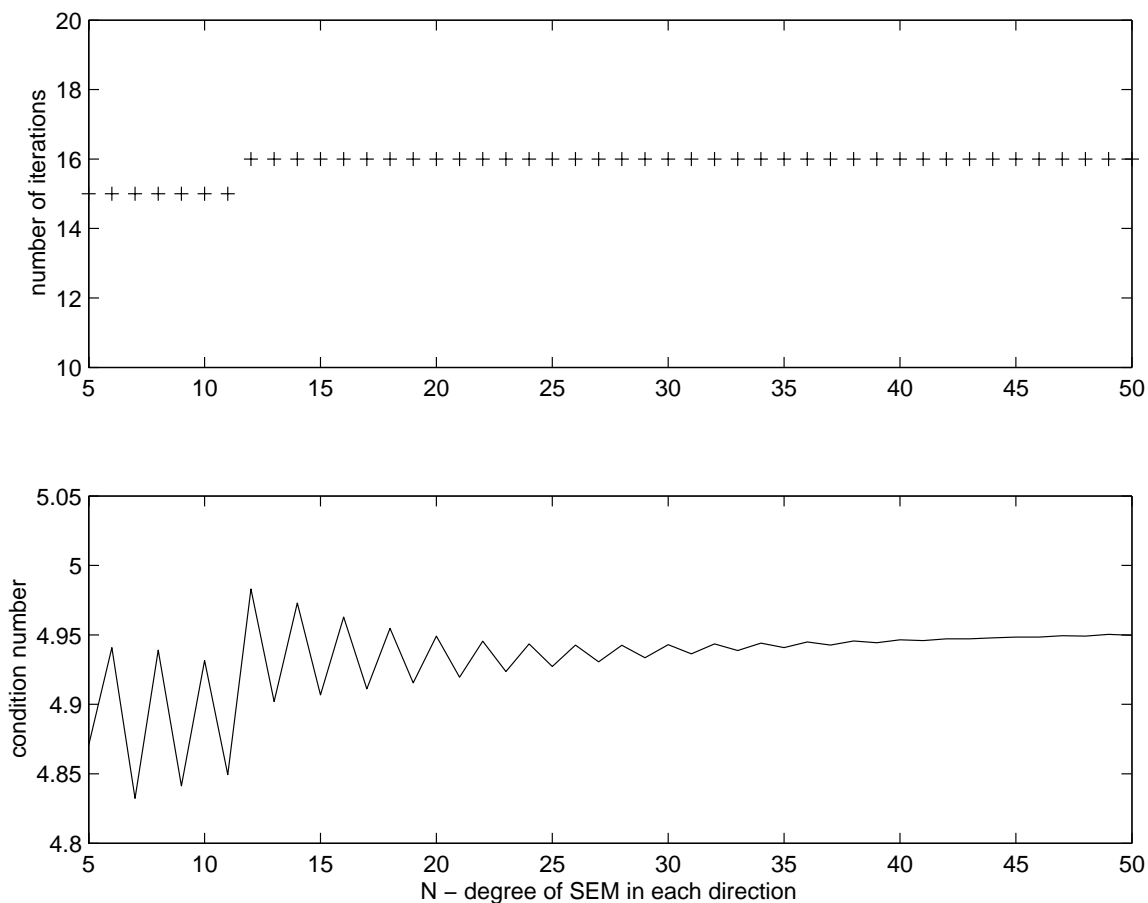
Domain decomposition methods: condition number bound

Fixed and generous overlap:

$$\kappa(T_{as2}) \leq C(N_c + 1)^2 \frac{\max(\alpha, \beta)}{\min(\alpha, \beta)}$$

Minimal overlap:

(vertex-centered: $\delta/h \sim N^{-1}$, $\gamma \leq 0.5$,
extended subdomain: $\delta/h \sim N^{-2}$, $\gamma \leq 1$)

$$\kappa(T_{as2}) \leq C(N_c + 1)^2 N^{\gamma}$$
$$\frac{\max(\alpha, \beta)}{\min(\alpha, \beta)} \left(1 + \left(\frac{H}{\delta}\right)^2\right)$$

Limit cases $\alpha \to 0$ and $\beta \to 0$ allow different bounds, independent of α or β, respectively.

Proof of the condition number estimate

- Uses the abstract Schwarz method framework [e.g., Smith et al '96]

- We use exact solvers, implying $\omega = 1$.

- Largest eigenvalue is bounded by number of colors N_C for overlapping subdomains (4 in the 2×2 case) plus one.

- Only part requiring work and thought: lower bound for smallest eigenvalue. Done by exhibiting splitting $\mathbf{u} = \sum \mathbf{u}_i$ and estimating (from above) C^2 in $\sum a(\mathbf{u}_i, \mathbf{u}_i) \leq C^2 a(\mathbf{u}, \mathbf{u})$

- Extension of Toselli [Numer. Math. '00] to spectral case (i.e., N-dependence)

Condition number estimates: required estimates

We reduced the N-dependence in the condition number estimate to the following three required estimates:

- Interpolation estimate on div-free H(curl) with polynomial curl:

$$||(I-\mathbf{\Pi}_N^{ND,I})\mathbf{w}||_0 \leq Chf_1(N)||\operatorname{\mathbf{curl}}\mathbf{w}||_0$$

- L^2-stability of local splitting:

$$||\mathbf{\Pi}_N^{ND,I}(\chi_i\mathbf{u})||_0 \leq Cf_2(N)||\chi_i\mathbf{u}||_0$$

- curl-stability of local splitting:

$$||\operatorname{\mathbf{curl}}\left(\mathbf{\Pi}_N^{ND,I}(\chi_i\mathbf{u})\right)||_0 \leq Cf_3(N)||\operatorname{\mathbf{curl}}(\chi_i\mathbf{u})||_0$$

  implied by L^2-stability of local splitting in a RT type space.

Domain decomposition methods: condition number bound

- $f_1(N) = 1 + C(\epsilon)N^{-1+\epsilon} \leq 1 + C(\epsilon)$. In two dimensions, and possibly (unproven) in three dimensions, $f_1(N) = C(\epsilon)N^{-1+f(\epsilon)}$.

- For generous overlap $f_2(N) = f_3(N) = 1$ (analytic and numerical result).

- For minimal overlap $\delta/h \sim N^{-2}$, $f_2(N) = f_3(N) = N^\gamma$, with $\gamma \leq 1$ (numerical result).

Inverse of smallest eigenvalue is bounded by:
$$\max\left(CN_c\left(1 + \frac{H}{\delta}\right), C\frac{\max(\alpha,\beta)}{\min(\alpha,\beta)}(1 + N_c f_2^2(N)),\right.$$
$$\left. C\frac{\max(\alpha,\beta)}{\min(\alpha,\beta)}\left\{1 + N_c f_3^2(N)\left(1 + \left(\frac{H + h f_1(N)}{\delta}\right)^2\right)\right\}\right).$$

In the moment we run extensive numerical tests to empirically determine the exponents of N and $\frac{H}{\delta}$ in the condition number, and try to prove the f_2, f_3 result for small overlap.

Work in progess, *planned extensions*

- Improve theory, prove more estimates.

- Implementing and analyzing other domain decomposition methods, such as iterative substructuring methods and *mortar elements*.

- Extending methods to three dimensions.

- *Extend methods to jumping or seperable or tensor α, β.*

- *Numerical tests for complex case, radition boundary conditions, indefinite case or high wave number.*

- *Implementation of mapped spectral elements.*